

2,5-Furandione  
108-31-6 | DTXSID7024166

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $2.17 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $3.17 \times 10^{-1}$

**Confidence level:**  $6.13 \times 10^{-1}$

## Nearest Neighbors from the Training Set

Image not found

2,5-Furandione

**Measured:**  $1.45 \times 10^{-12}$

**Predicted:**  $2.17 \times 10^{-12}$

Image not found

Glyoxal

**Measured:**  $1.14 \times 10^{-11}$

**Predicted:**  $1.14 \times 10^{-11}$

Image not found

2(3H)-Furanone

**Measured:**  $4.45 \times 10^{-11}$

**Predicted:**  $3.74 \times 10^{-11}$